

# Effective Hamiltonians with Relativistic Corrections

## *II) Application to Compton Scattering by a Proton*

S. Scherer, G. I. Poulis and H. W. Fearing

TRIUMF, Vancouver, British Columbia, Canada V6T 2A3

### **Abstract**

We discuss two different methods of obtaining “effective  $2 \times 2$  Hamiltonians” of the electromagnetic interaction which include relativistic corrections. One is the standard Foldy–Wouthuysen transformation which we compare with the Hamiltonian obtained from a direct reduction of the matrix element of the interaction Hamiltonian between positive–energy solutions of the free Dirac equation. The two approaches are applied to Compton scattering by a proton for which a low–energy theorem exists. It is found that the Foldy–Wouthuysen Hamiltonian yields the same result as a covariant calculation. This is not true for the direct reduction method which will in general lead to incorrect results even after restoring the gauge invariance property of the Hamiltonian. Furthermore, it is shown that an identification of the Z–diagrams of the usual Dirac representation with the contact graphs of the Foldy–Wouthuysen representation is incorrect beyond the order of the low–energy theorem.

## **1 Introduction**

The use of “effective  $2 \times 2$  Hamiltonians” for relativistic corrections is one of the main ingredients of many calculations in low– and intermediate–energy nuclear physics. For the electromagnetic interaction of the nucleon such correction terms beyond the standard Pauli–Hamiltonian [1, 2] are conventionally generated through a Foldy–Wouthuysen transformation [2, 3, 4].

In some applications the Foldy–Wouthuysen transformation is applied to a Hamiltonian containing strong interactions as well [5, 6, 7]. The algorithm [2, 3, 4] consists of successive applications of unitary transformations of the wave functions. It provides a systematic procedure to block–diagonalize the Hamiltonian order by order in  $1/M$ , leading to a decoupling of positive– and negative–energy states to any desired order in  $1/M$ . As the unitary transformations used are in general time–dependent, the old and the new Hamiltonian are not unitarily equivalent [8, 9]. The new Hamiltonian rather contains an additional piece involving the unitary transformation and the time derivative of the inverse transformation. Nevertheless, such an approach automatically leads to the same result for the S–matrix as the standard covariant calculation [10].

In a second approach the matrix element of the interaction Hamiltonian is evaluated between positive–energy solutions of the free Dirac equation. The result is then interpreted as the matrix element of some effective Hamiltonian between two–component Pauli spinors. The so constructed Hamiltonian is then used in conventional old–fashioned time–ordered perturbation theory.

In ref. [10] we have studied for a generic interaction how the two methods compare and when they are expected to give different results. We have seen that it is important to investigate processes which require higher than first–order perturbation theory. It is the purpose of this work to apply the different methods to a specific process, namely low–energy Compton scattering by a proton, in order to make more quantitative statements. For several reasons Compton scattering provides an ideal process to test the approaches mentioned above. First of all, when expanded in a power series in the frequency  $\omega$  of the photon, the two leading terms of the T–matrix are determined by a low–energy theorem [11, 12]. The coefficients of the series are expressed in terms of on–shell properties of the proton, namely its mass, charge and anomalous magnetic moment. The derivation of this theorem is based on gauge and relativistic invariance. Secondly, it was shown in ref. [11] that a covariant calculation of the s– and u–channel Born terms using the interaction Hamiltonian for a Dirac particle with an anomalous magnetic moment as proposed by Pauli [2, 13] reproduces the low–energy theorem. Finally, we can address the important question of gauge invariance which will in general impose some restrictions on the construction of effective Hamiltonians.

Alternatively we could have considered pion photoproduction at threshold where two different interactions, namely the strong and the electromagnetic,

enter and a low-energy theorem exists as well [14, 15, 16, 17]. However, the observations for that process are very similar and all the relevant points can be made using Compton scattering.

Our paper is organized as follows. In the next section we will define the interaction Hamiltonians which are used in section 3 to calculate the T-matrix in second-order perturbation theory. We will discuss the results to order  $\omega^2/M^3$  and comment on gauge invariance. Finally, in section 4 we will give a short summary.

## 2 Definition of the Interaction Hamiltonians

In this section we will define the different interaction Hamiltonians which we will use to calculate the corresponding T-matrix element for low-energy Compton scattering to order  $1/M^3$ .

### 2.1 Relativistic Hamiltonian

For the relativistic description we will work with the Dirac equation describing the interaction of a Dirac proton having an anomalous magnetic moment ( $\kappa = 1.79$ ) with an external electromagnetic field,

$$i\frac{\partial\Psi(x)}{\partial t} = (H_0 + H_I(t))\Psi(x), \quad (1)$$

where  $H_0 = \vec{\alpha} \cdot \vec{p} + \beta M$  is the free Dirac Hamiltonian and  $H_I(t)$  is given by [2, 13]

$$H_I(t) = \beta(eA^\mu\gamma_\mu - \frac{e\kappa}{4M}\sigma_{\mu\nu}F^{\mu\nu}), \quad (2)$$

with  $F^{\mu\nu} = \partial^\nu A^\mu - \partial^\mu A^\nu$ . A calculation involving the model Hamiltonian of eq. (2) obviously cannot take *all* strong interaction effects into account, such as, e. g. , off-shell effects [18, 19, 20] or transitions to excited states. However, for our purposes this is not required, as we only want to use the second-order covariant calculation as a reference, which defines the “correct” relativistic result within the framework of the model Hamiltonian.

## 2.2 The Foldy–Wouthuysen Hamiltonian

The Foldy–Wouthuysen transformation [2, 3, 4] provides a method which order by order in  $1/M$  decouples the upper from the lower components. We apply the procedure to the Hamiltonian of eq. (1) to obtain a representation of the  $4 \times 4$  Hamiltonian which is block-diagonal to order  $1/M^3$  [10]. We define the upper left-hand block of the  $4 \times 4$  Foldy–Wouthuysen Hamiltonian as the effective  $2 \times 2$  Hamiltonian,  $H^{eff-FW}$ , to be used in our calculation of Compton scattering by the proton in second-order perturbation theory. We keep interaction terms up to second order in the coupling constant  $e$  and obtain,

$$i \frac{\partial \Psi(x)}{\partial t} = (H_0^{eff-FW} + H_1^{eff-FW}(t) + H_2^{eff-FW}(t)) \Psi(x), \quad (3)$$

with

$$\begin{aligned} H_0^{eff-FW} &= M + \frac{\vec{p}^2}{2M} - \frac{\vec{p}^4}{8M^3}, \\ H_1^{eff-FW}(t) &= e\Phi - \frac{e}{2M}(\vec{p} \cdot \vec{A} + \vec{A} \cdot \vec{p}) - \frac{e}{2M}(1 + \kappa)\vec{\sigma} \cdot \vec{B} \\ &\quad - i \frac{e(1 + 2\kappa)}{8M^2}[\vec{\sigma} \cdot \vec{p}, \vec{\sigma} \cdot \vec{E}] - \frac{e\kappa}{16M^3}\{\vec{\sigma} \cdot \vec{p}, \vec{\sigma} \cdot \dot{\vec{E}}\} \\ &\quad + \frac{e}{8M^3}\{\vec{p}^2, \{\vec{\sigma} \cdot \vec{p}, \vec{\sigma} \cdot \vec{A}\}\} + \frac{e\kappa}{16M^3}\{\vec{\sigma} \cdot \vec{p}, \{\vec{\sigma} \cdot \vec{p}, \vec{\sigma} \cdot \vec{B}\}\}, \\ H_2^{eff-FW}(t) &= \frac{e^2 \vec{A}^2}{2M} + \frac{e^2}{4M^2}(1 + 2\kappa)\vec{\sigma} \cdot \vec{E} \times \vec{A} + \frac{e^2}{8M^3}(1 + \kappa + \kappa^2)\vec{E}^2 \\ &\quad - \frac{e^2}{8M^3}(\vec{p}^2 \vec{A}^2 + \vec{A}^2 \vec{p}^2 + 4\vec{p} \cdot \vec{A} \vec{A} \cdot \vec{p} + (\vec{\nabla} \cdot \vec{A})^2 + \vec{B}^2 \\ &\quad - 2i\vec{p} \cdot \vec{A} \vec{\nabla} \cdot \vec{A} + 2i\vec{\nabla} \cdot \vec{A} \vec{A} \cdot \vec{p} + 2\vec{p} \cdot \vec{A} \vec{\sigma} \cdot \vec{B} + 2\vec{\sigma} \cdot \vec{B} \vec{A} \cdot \vec{p}) \\ &\quad - \frac{e^2 \kappa}{8M^3}(\vec{\sigma} \cdot \vec{p} \vec{A} \cdot \vec{B} + \vec{A} \cdot \vec{B} \vec{\sigma} \cdot \vec{p} + \vec{\sigma} \cdot \vec{A} \vec{B} \cdot \vec{p} + \vec{p} \cdot \vec{B} \vec{\sigma} \cdot \vec{A} \\ &\quad + \vec{A} \cdot \vec{\nabla} \times \vec{B} - \vec{A} \cdot \dot{\vec{E}}), \end{aligned} \quad (4)$$

where  $\vec{E} = -\vec{\nabla}\Phi - \dot{\vec{A}}$  and  $\vec{B} = \vec{\nabla} \times \vec{A}$  and  $\dot{\mathcal{O}}$  refers to  $\partial \mathcal{O} / \partial t$ . Note that  $\Psi(x)$  in eq. (3) denotes a two-component wave function.

### 2.3 Direct Pauli Reduction Hamiltonian

In many applications a different method is used to obtain an effective  $2 \times 2$  Hamiltonian. Given a general relativistic interaction, it consists of evaluating the matrix element of the interaction operator between free positive-energy solutions of the Dirac equation and reducing it to two-component form. The result may then be expanded in a power series in  $1/M$  and is interpreted as an effective operator to be used with a free Hamiltonian  $H_0^{eff-P}$ . Applying this procedure to the interaction Hamiltonian of eq. (2) and keeping only terms to order  $1/M^3$  yields the following Schrödinger equation

$$i \frac{\partial \Psi(x)}{\partial t} = (H_0^{eff-P} + H_I^{eff-P}(t)) \Psi(x), \quad (5)$$

with  $H_0^{eff-P}$  the same as  $H_0^{eff-FW}$  in eq. (4) and

$$\begin{aligned} H_I^{eff-P}(t) = & e\Phi - \frac{e}{2M}(\vec{p} \cdot \vec{A} + \vec{A} \cdot \vec{p}) - \frac{e}{2M}(1 + \kappa)\vec{\sigma} \cdot \vec{B} \\ & - \frac{e}{8M^2}[\vec{\sigma} \cdot \vec{p}, [\vec{\sigma} \cdot \vec{p}, \Phi]] - i \frac{e\kappa}{4M^2}[\vec{\sigma} \cdot \vec{p}, \vec{\sigma} \cdot \vec{E}] \\ & + \frac{e}{8M^3}\{\vec{p}^2, \{\vec{\sigma} \cdot \vec{p}, \vec{\sigma} \cdot \vec{A}\}\} + \frac{e}{16M^3}[\vec{p}^2, [\vec{\sigma} \cdot \vec{p}, \vec{\sigma} \cdot \vec{A}]] \\ & + \frac{e\kappa}{16M^3}\{\vec{\sigma} \cdot \vec{p}, \{\vec{\sigma} \cdot \vec{p}, \vec{\sigma} \cdot \vec{B}\}\}. \end{aligned} \quad (6)$$

The  $2 \times 2$  effective interaction Hamiltonian  $H_I^{eff-P}$  of eq. (6) may be interpreted as the upper left-hand block of the transformed operator  $H_I^P = T_0 H_I T_0^\dagger$ , where  $T_0$  denotes the time-independent free Foldy-Wouthuysen transformation (see e. g. eq. (8) of ref. [10]). We emphasize that  $H_I^P$  is not block-diagonal, i. e. , it will connect positive- and negative-energy eigenstates of the free Foldy-Wouthuysen Hamiltonian.

The above procedure only produces a *linear* interaction term and no contact interactions. However, it is well-known that a gauge-invariant coupling through a minimal substitution in  $H_0^{eff-P}$  generates linear and quadratic (and higher-order) terms in  $\vec{A}$  as required by gauge invariance. As such terms are absent in the Hamiltonian of eq. (5) it will not exhibit the correct transformation behavior under a gauge transformation. Of course, we can cure this problem by introducing additional interaction terms by hand, such that the resulting Hamiltonian transforms properly. However, we have to

keep in mind that one of our main purposes in considering Compton scattering is a *critical* examination of the use of effective Hamiltonians. In fact, for interactions other than the electromagnetic, there is in general *no* guiding principle which tells us whether or not the simple matrix element reduction is a reasonable procedure to generate an effective Hamiltonian. For that reason we will nevertheless use the Hamiltonian of eq. (6) (being aware that this will lead to unacceptable results) and will postpone the question of gauge invariance until we discuss our results.

### 3 Calculation of the T–Matrix Element

In this section we will calculate the T–matrix element for low–energy Compton scattering in second–order perturbation theory using the different interaction Hamiltonians of section 2, eq. (2), (4) and (6), and compare the results.

The kinematical variables and polarization vectors for Compton scattering are defined in figure 1. The calculations are performed in the laboratory frame, where the energies  $\omega$  and  $\omega'$  of the initial and final photon are related by

$$\omega' = \omega \left( 1 + \frac{\omega}{M}(1 - \cos(\theta)) \right)^{-1} = \omega \left( 1 - \frac{\omega}{M}(1 - \cos(\theta)) + \left[ \frac{\omega^2}{M^2} \right] \right). \quad (7)$$

In eq. (7)  $\theta$  denotes the angle between the momenta of the initial and the final photon in the laboratory system and  $[\omega^2/M^2]$  means “of order of  $\omega^2/M^2$ ”. Furthermore, we make use of the radiation gauge,  $\Phi = 0, \vec{\nabla} \cdot \vec{A} = 0$ . We express the result as an operator which still has to be evaluated between two–component Pauli spinors of the proton. Any calculation of the T–matrix element<sup>1</sup> to order  $1/M^3$  may be written in the following form [12, 21]

$$\begin{aligned} t_{fi} = & \vec{\epsilon} \cdot \vec{\epsilon}' A_1 + i\vec{\sigma} \cdot \vec{\epsilon}' \times \vec{\epsilon} A_2 + \hat{k}' \times \vec{\epsilon}' \cdot \hat{k} \times \vec{\epsilon} A_3 + i\vec{\sigma} \cdot (\hat{k}' \times \vec{\epsilon}') \times (\hat{k} \times \vec{\epsilon}) A_4 \\ & + i\hat{k} \cdot \vec{\epsilon}' \vec{\sigma} \cdot \hat{k} \times \vec{\epsilon} A_5 + i\hat{k}' \cdot \vec{\epsilon} \vec{\sigma} \cdot \hat{k}' \times \vec{\epsilon}' A_6 \\ & + i\hat{k} \cdot \vec{\epsilon}' \vec{\sigma} \cdot \hat{k}' \times \vec{\epsilon} A_7 + i\hat{k}' \cdot \vec{\epsilon} \vec{\sigma} \cdot \hat{k} \times \vec{\epsilon}' A_8, \end{aligned} \quad (8)$$

---

<sup>1</sup>The T–matrix element  $t_{fi}$  is related to the invariant amplitude  $\mathcal{M}$  of ref. [2] through  $t_{fi} = -i(M/\sqrt{E_i E_f})\mathcal{M}$ .

where  $\hat{k}, \vec{\epsilon}(\hat{k}', \vec{\epsilon}')$  refer to the direction and the polarization of the initial (final) photon, respectively<sup>2</sup>. In the following we will calculate the amplitudes  $A_i$  as predicted to second-order perturbation theory using the different Hamiltonians.

### 3.1 Covariant Calculation

In the covariant calculation the invariant amplitude to second-order perturbation theory using the Hamiltonian of eq. (2) reads

$$\begin{aligned} \mathcal{M} = & -ie^2 \bar{u}(p_f) \left( \not{\epsilon}' - \frac{\kappa}{2M} \not{k}' \not{\epsilon}' \right) \frac{1}{\not{p}_i + \not{k} - M + i\delta} \left( \not{\epsilon} + \frac{\kappa}{2M} \not{k} \not{\epsilon} \right) u(p_i) \\ & + (\epsilon \leftrightarrow \epsilon', k \leftrightarrow -k'), \end{aligned} \quad (9)$$

where the expression for the u-channel diagram may be obtained from the s-channel diagram through crossing symmetry [2] as indicated in eq. (9). In eq. (9) we have introduced  $-i\delta$  instead of the standard  $-i\epsilon$  as the small imaginary mass required by the Feynman–Stückelberg boundary condition in order to avoid confusion with the polarization vector  $\epsilon^\mu$ .

For our discussion it turns out to be useful to split the Feynman propagator of the nucleon,  $S_F(p)$ , into its positive- and negative-frequency contribution,

$$\begin{aligned} S_F(p) &= \frac{1}{\not{p} - m + i\delta} \\ &= S_F^{(+)}(p) + S_F^{(-)}(p) \\ &= \frac{E\gamma^0 - \vec{p} \cdot \vec{\gamma} + M}{2E(p^0 - E + i\delta)} + \frac{E\gamma^0 + \vec{p} \cdot \vec{\gamma} - M}{2E(p^0 + E - i\delta)}, \end{aligned} \quad (10)$$

with  $E = \sqrt{\vec{p}^2 + M^2}$ . Such a separation allows one to identify Z-diagrams and ordinary diagrams of old-fashioned time-ordered perturbation theory (see e. g. ref. [23] and figure 2). It should, however, be noted that, although the individual diagrams of covariant perturbation theory are Lorentz scalars, this is not separately true for their positive- and negative-frequency contributions [23]. In other words, these contributions are frame-dependent

---

<sup>2</sup>It is possible to construct a generalized Hamiltonian which parameterizes the T-matrix including all strong interaction effects to order  $\omega^2/M^3$  [21, 22]. Such an effective Hamiltonian involves the Compton polarizabilities  $\bar{\alpha}$  and  $\bar{\beta}$ .

quantities. Furthermore, as was pointed out in ref. [24], the notion of Z-diagrams depends on the interaction as well as the representation used. Here, we will refer to Z-diagrams (ordinary diagrams) as those resulting from the negative- (positive-) frequency part of the propagator of eq. (10) when using the Hamiltonian of eq. (2).

After inserting eq. (10) into eq. (9) we expand the resulting expression in  $1/M$  and bring it into the form of eq. (8). The predictions of this straightforward but tedious calculation for the amplitudes  $A_i$  separated into their forward and backward contributions are tabulated in table 1 and 2.

### 3.2 Foldy–Wouthuysen Calculation

The calculation involving the effective Foldy–Wouthuysen Hamiltonian of eq. (4) is performed in second-order time-ordered perturbation theory and the contribution to the S-matrix of second order in the coupling constant reads

$$\begin{aligned}
S_{fi} = & -2\pi i \delta(E_f + \omega' - E_i - \omega) \left\{ \langle \Phi_{0f}^{FW} | H_2^{eff-FW} | \Phi_{0i}^{FW} \rangle \right. \\
& + \sum_{spins} \int d^3p \frac{\langle \Phi_{0f}^{FW} | H_{1em}^{eff-FW} | \Phi_{0\vec{p}}^{FW} \rangle \langle \Phi_{0\vec{p}}^{FW} | H_{1abs}^{eff-FW} | \Phi_{0i}^{FW} \rangle}{E_f + \omega' - E_{\vec{p}} + i\delta} \\
& \left. + \sum_{spins} \int d^3p \frac{\langle \Phi_{0f}^{FW} | H_{1abs}^{eff-FW} | \Phi_{0\vec{p}}^{FW} \rangle \langle \Phi_{0\vec{p}}^{FW} | H_{1em}^{eff-FW} | \Phi_{0i}^{FW} \rangle}{E_f - \omega - E_{\vec{p}} + i\delta} \right\}.
\end{aligned} \tag{11}$$

In arriving at eq. (11) we have assumed a harmonic time dependence for the interaction, i. e. ,  $\exp(-i\omega t)$  and  $\exp(i\omega' t)$  for the initial and final photon appearing in the interaction Hamiltonian of eq. (4), respectively. Furthermore,  $H_{1em}^{eff-FW}$  and  $H_{1abs}^{eff-FW}$  refer to the emission and absorption of a photon, respectively, and it is understood that the part of  $H_2^{eff-FW}$  which at the same time creates and annihilates a photon is used. The Hamiltonian  $H_2^{eff-FW}$  gives rise to a contact term, whereas  $H_1^{eff-FW}$  contributes “quadratically” in second-order perturbation theory (see figure 3). In Coulomb gauge, the leading-order term of  $H_1^{eff-FW}$  is of order  $1/M$ . As we are interested in the T-matrix element to order  $1/M^3$ , we need the linear interaction Hamiltonian



to order  $1/M^2$  only<sup>3</sup>. Establishing the graphical rules corresponding to the interaction Hamiltonians of eq. (4) is straightforward, but the expressions are lengthy. We only report the predictions for the amplitudes  $A_i$  in table 1 and 2, separated according to their origin as contact or non-contact terms.

### 3.3 Calculation Involving the Effective Hamiltonian $H_I^{eff-P}$ and Gauge Invariance

Finally, a second-order calculation involving the effective Hamiltonian of eq. (6),  $H_I^{eff-P}$ , gives rise to

$$S_{fi} = -2\pi i \delta(E_f + \omega' - E_i - \omega) \times \left\{ \sum_{spins} \int d^3p \frac{\langle \Phi_{0f}^{FW} | H_{Iem}^{eff-P} | \Phi_{0\vec{p}}^{FW} \rangle \langle \Phi_{0\vec{p}}^{FW} | H_{Iabs}^{eff-P} | \Phi_{0i}^{FW} \rangle}{E_f + \omega' - E_{\vec{p}} + i\delta} + \sum_{spins} \int d^3p \frac{\langle \Phi_{0f}^{FW} | H_{Iabs}^{eff-P} | \Phi_{0\vec{p}}^{FW} \rangle \langle \Phi_{0\vec{p}}^{FW} | H_{Iem}^{eff-P} | \Phi_{0i}^{FW} \rangle}{E_f - \omega - E_{\vec{p}} + i\delta} \right\}. \quad (12)$$

As we have seen in ref. [10] such a calculation amounts to neglecting the negative-frequency part of the covariant calculation. Thus we already know the results for the  $A_i$ , as we have split the covariant calculation into its forward and backward part.

Approximations, such as the neglect of the negative-energy contributions, will in general be in conflict with gauge invariance. Thus we have to address the gauge invariance property of the equation of motion<sup>4</sup>

$$i \frac{\partial \Psi(x)}{\partial t} = H(\Phi, \vec{A}) \Psi(x). \quad (13)$$

Gauge invariance means that

$$\Psi'(x) = \exp(-ie\chi(x)) \Psi(x) \quad (14)$$

---

<sup>3</sup>If one wants to check gauge invariance to order  $1/M^3$  one has to retain terms to order  $1/M^3$  in  $H_1^{eff-FW}$ , since the leading-order term in  $H_1^{eff-FW}$  is proportional to  $\Phi$ .

<sup>4</sup>Although we only write down the potentials  $\Phi$  and  $\vec{A}$  as the argument of the Hamiltonian, it is understood that it may as well depend on derivatives of the potentials.

is a solution of

$$i \frac{\partial \Psi'(x)}{\partial t} = H(\Phi + \dot{\chi}, \vec{A} - \vec{\nabla} \chi) \Psi'(x), \quad (15)$$

provided  $\Psi(x)$  is a solution of eq. (13) [25]. From this we may derive the following constraint for the form of the Hamiltonian

$$H(\Phi + \dot{\chi}, \vec{A} - \vec{\nabla} \chi) - \exp(-ie\chi) H(\Phi, \vec{A}) \exp(ie\chi) - e\dot{\chi} = 0. \quad (16)$$

The effective Foldy–Wouthuysen Hamiltonian of eq. (3) satisfies the gauge invariance property to order  $e^2$  whereas the effective Hamiltonian of eq. (5) is not gauge-invariant even to first order in  $e$ . Suppose we denoted the effective Hamiltonian of eq. (5) by  $H_A$  and we wanted to add a Hamiltonian  $H_B$  such that the sum satisfied the condition of eq. (16). Inserting  $H_A + H_B$  into eq. (16) it is easily seen that the condition for  $H_B$  reads

$$\begin{aligned} \exp(-ie\chi) H_B(\Phi, \vec{A}) \exp(ie\chi) - H_B(\Phi + \dot{\chi}, \vec{A} - \vec{\nabla} \chi) = \\ H_A(\Phi + \dot{\chi}, \vec{A} - \vec{\nabla} \chi) - \exp(-ie\chi) H_A(\Phi, \vec{A}) \exp(ie\chi) - e\dot{\chi}. \end{aligned} \quad (17)$$

From eq. (17) it is seen that  $H_B$  cannot be determined uniquely as one may always add another term  $H_C$  which separately satisfies

$$\exp(-ie\chi) H_C(\Phi, \vec{A}) \exp(ie\chi) - H_C(\Phi + \dot{\chi}, \vec{A} - \vec{\nabla} \chi) = 0. \quad (18)$$

Let us for convenience consider eq. (5) to order  $1/M^2$  only, as this is sufficient for the point we want to make. Inserting  $H_A = H_0^{eff-P} + H_I^{eff-P}$  into eq. (17) we obtain the following constraint for  $H_B$

$$\begin{aligned} \exp(-ie\chi) H_B(\Phi, \vec{A}) \exp(ie\chi) - H_B(\Phi + \dot{\chi}, \vec{A} - \vec{\nabla} \chi) = \\ -\frac{e}{8M^2} [\vec{\sigma} \cdot \vec{p}, [\vec{\sigma} \cdot \vec{p}, \dot{\chi}]] + \frac{e^2}{2M} (2\vec{A} \cdot \vec{\nabla} \chi - (\vec{\nabla} \chi)^2) \\ -\frac{ie^2}{8M^2} [\chi, [\vec{\sigma} \cdot \vec{p}, [\vec{\sigma} \cdot \vec{p}, \Phi]]] + \frac{e^2 \kappa}{4M^2} [\chi, [\vec{\sigma} \cdot \vec{p}, \vec{\sigma} \cdot \vec{E}]] + [e^3]. \end{aligned} \quad (19)$$

From the right-hand side of eq. (19) we can now see that  $H_0^{eff-P} + H_I^{eff-P}$  does not satisfy the constraint of eq. (16) even to leading order in  $e$ . The introduction of e. g.

$$H_B(\Phi, \vec{A}) = \frac{e}{8M^2} [\vec{\sigma} \cdot \vec{p}, [\vec{\sigma} \cdot \vec{p}, \Phi]] + \frac{e^2 \vec{A}^2}{2M} + \frac{ie^2 \kappa}{4M^2} [\vec{\sigma} \cdot \vec{A}, \vec{\sigma} \cdot \vec{E}] \quad (20)$$

makes the sum  $H_A + H_B$  transform according to eq. (16) to order  $e^2$  and  $1/M^2$ . The second term of eq. (20) “completes” the minimal substitution in the kinetic-energy term of eq. (5) to the order we are considering here. The other two terms are clearly not unique and a comparison with the Foldy–Wouthuysen Hamiltonian to the same order, namely  $1/M^2$ , shows that the two Hamiltonians are in fact different.

### 3.4 Results and Discussion

In table 1 we show the results for the amplitudes  $A_i$  to the order of the low-energy theorem, namely  $[1/M]$  and  $[\omega/M^2]$ . We find that the negative-frequency contribution of the covariant calculation (Z-diagrams) yields exactly the same result as the contact interaction of the Foldy–Wouthuysen transformation. Similarly, we have as well a correspondence between the positive-frequency part (ordinary diagrams) on the one hand and the non-contact terms of the FW calculation on the other hand.

The *naive* – but within the framework of nonrelativistic second-order perturbation theory consistent – calculation involving the effective Hamiltonian of eq. (6) is identical with the positive-frequency contribution of the covariant calculation and leads to completely unacceptable results. Even the leading-order term, the so-called Thomson limit, is not reproduced. Inspection of table 1 tells us that the neglect of the negative-frequency contribution is responsible for such behavior. Such an approximation will spoil the gauge invariance property of the model. However, it is well known that the low-energy theorem for the Thomson limit is based on gauge invariance. For that reason we constructed an additional interaction term to make the total Hamiltonian gauge-invariant. This construction naturally involved the  $e^2 \vec{A}^2/2M$  term which then generated the correct Thomson limit. However, the other terms are by no means unique. As we can see from table 1 even including the additional Hamiltonian  $H_B$  of eq. (20) does not reproduce the correct low-energy theorem prediction beyond the leading-order term, although the Hamiltonian used is gauge-invariant to order  $e^2$ . It was pointed out by Low [12] that the determination of the terms beyond the Thomson limit require more input than gauge invariance alone. Our example clearly is in agreement with this observation. In other words, enforcing gauge invariance is required to obtain the Thomson limit, but it does not predict the next-to-leading-order term of the low-energy theorem.

The Compton scattering by a proton firstly demonstrates how misleading it may be to use effective Hamiltonians obtained from a two-component reduction of a relativistic matrix element. The failure to reproduce the contributions of the Z-diagrams originates from the fact that the  $2 \times 2$  effective Hamiltonian  $H_I^{eff-P}$  is generated from a  $4 \times 4$  Hamiltonian  $H_I^P$  which is *not* block-diagonal. Use of  $H_I^{eff-P}$  then amounts to a truncation of the Hilbert space, namely the neglect of negative-energy states in this approach, which will in general lead to unreliable results. In contrast, the  $4 \times 4$  Foldy-Wouthuysen Hamiltonian  $H^{FW}$  is block-diagonal and hence using the  $2 \times 2$  Hamiltonian  $H^{eff-FW}$  does not make a difference, as  $H^{FW}$  does not connect positive- and negative-energy states in the FW representation.

Furthermore, we have seen that gauge invariance alone is in general not sufficient to overcome this shortcoming, i. e. , to determine more than the leading-order term. For a similar discussion of the second point within the framework of a quantum field theoretical model see ref. [26].

The terms of order  $\omega^2/M^3$  are beyond the prediction of the low-energy theorem and hence are model-dependent. The results of the covariant calculation and the Foldy-Wouthuysen calculation for these terms are listed in table 2. Once again we see that the *total* result of both calculations is the same at this order in agreement with our observations in ref. [10]. However, from table 1 one might have concluded that the correspondence between Z-diagrams and contact interactions and equally between ordinary diagrams and non-contact terms holds true for higher orders in  $1/M$  as well. It can now be seen that for some of the amplitudes  $A_i$  this is no longer true. In order to be specific, we find that the Z-diagram contribution to the amplitudes  $A_1$ ,  $A_5$  and  $A_6$  differs from the contact terms.

As in table 1 the result of the effective Hamiltonian is given by the positive-frequency part of the covariant calculation. We have not made the effort of forcing the effective Hamiltonian to be gauge-invariant to order  $e^2$  and  $1/M^3$  since the result will not be unique anyway.

## 4 Summary and Conclusions

In this work we considered Compton scattering by the proton within three different approaches. Firstly, we performed a covariant calculation to second-order perturbation theory. In order to identify Z-diagrams and ordinary

diagrams in the covariant approach, we split the Feynman propagator into its positive- and negative-frequency contribution. We expanded the so obtained T-matrix element to order  $\omega^2/M^3$  and used the result as a reference for the nonrelativistic calculations with effective Hamiltonians.

The calculation involving the Foldy-Wouthuysen Hamiltonian correctly reproduced the reference result of the covariant approach. This was expected as the  $4 \times 4$  Foldy-Wouthuysen Hamiltonian is block-diagonal and thus does not couple between positive- and negative-energy states. The neglect of the negative-energy states in going from the full S-matrix to the effective one has no consequence and hence the full (and as a reference correct) S-matrix is still reproduced. However, we saw that an identification of the Z-diagrams with the contact interaction of the Foldy-Wouthuysen Hamiltonian is *not* correct beyond the order of the low-energy theorem.

Finally, the effective Hamiltonian  $H_I^{eff-P}$  obtained from a direct reduction of the relativistic interaction Hamiltonian between positive-energy solutions of the free Dirac equation led to incorrect results. The reason is that  $H_I^{eff-P}$  is derived as the upper left-hand block from a  $4 \times 4$  interaction Hamiltonian which is not block-diagonal. In this case, the neglect of the negative-frequency solutions makes a considerable difference. Even the leading-order term is not reproduced. This may be cured in part by enforcing the gauge invariance property of the corresponding Hamiltonian. However, as we saw, such a procedure is not unique, and thus there will always be some degree of arbitrariness involved, when enforcing gauge invariance.

## 5 Acknowledgements

This work was supported in part by a grant from the Natural Sciences and Engineering Research Council of Canada. The authors would like to thank B. K. Jennings for useful discussions.

## References

- [1] W. Pauli, General Principles of Quantum Mechanics, Springer, Berlin, 1980

- [2] J. D. Bjorken and S. D. Drell, Relativistic Quantum Mechanics, McGraw–Hill, New York, 1964
- [3] L. L. Foldy and S. A. Wouthuysen, Phys. Rev. **78** (1950) 29
- [4] C. Itzykson and J.-B. Zuber, Quantum Field Theory, McGraw–Hill, New York, 1980
- [5] J. L. Friar, Phys. Lett. **B59** (1975) 145
- [6] H. Hyuga and M. Gari, Nucl. Phys. **A274** (1976) 333
- [7] H. Göller and H. Arenhövel, Johannes Gutenberg-Universität, Mainz, preprint MKPH-T-92-3 (1992)
- [8] M. M. Nieto, Phys. Rev. Lett. **38** (1977) 1042
- [9] T. Goldman, Phys. Rev. **D15** (1977) 1063
- [10] H. W. Fearing, G. Poulis and S. Scherer, TRIUMF preprint 93-12 (1993)
- [11] M. Gell–Mann and M. L. Goldberger, Phys. Rev. **96** (1954) 1433
- [12] F. E. Low, Phys. Rev. **96** (1954) 1428
- [13] W. Pauli, Rev. Mod. Phys. **13** (1941) 203
- [14] N. M. Kroll and M. A. Ruderman, Phys. Rev. **93** (1954) 233
- [15] P. de Baenst, Nucl. Phys. **B24** (1970) 633
- [16] H. W. L. Naus, J. H. Koch and J. L. Friar, Phys. Rev. **C41** (1990) 2852
- [17] S. Scherer, J. H. Koch and J. L. Friar, NIKHEF–K preprint 92 - P8, to be published in Nucl. Phys. **A**
- [18] A. M. Bincer, Phys. Rev. **118** (1960) 855
- [19] E. M. Nyman, Nucl. Phys. **A154** (1970) 97
- [20] H. W. L. Naus and J. H. Koch, Phys. Rev. **C36** (1987) 2459

- [21] V. A. Petrun'kin and A. I. L'vov, Talk at 8th Intern. Seminar on Electromagnetic Interactions of Nuclei at Low and Medium Energies, Moscow, Dec. 2-5, 1991
- [22] A. I. L'vov, P. N. Lebedev Physical Institute, Moscow, Report No. 344 (1987) unpublished
- [23] S. Weinberg, Phys. Rev. **150** (1966) 1313
- [24] B. K. Jennings and C. Bennhold, TRIUMF preprint 92-26 (1992)
- [25] A. Messiah, Quantum Mechanics, Vol. I, North-Holland, Amsterdam, 1962
- [26] J. W. Bos, S. Scherer and J. H. Koch, Nucl. Phys. **A547** (1992) 488

	covariant calculation			FW calculation in s. o. p. t.	
amplitude	negative	positive	$H_B$	contact	non-contact
$A_1$	$\frac{1}{M}$	0	$\frac{1}{M}$	$\frac{1}{M}$	0
$A_2$	$-\frac{(\omega+\omega')(1+2\kappa)}{4M^2}$	0	$-\frac{(\omega+\omega')\kappa}{2M^2}$	$-\frac{(\omega+\omega')(1+2\kappa)}{4M^2}$	0
$A_4$	0	$\frac{(\omega+\omega')(1+\kappa)^2}{4M^2}$	0	0	$\frac{(\omega+\omega')(1+\kappa)^2}{4M^2}$
$A_5$	0	$\frac{\omega(1+\kappa)}{2M^2}$	0	0	$\frac{\omega(1+\kappa)}{2M^2}$
$A_6$	0	$-\frac{\omega'(1+\kappa)}{2M^2}$	0	0	$-\frac{\omega'(1+\kappa)}{2M^2}$

**Table 1: Compton Scattering amplitudes**

Contribution to the amplitudes  $A_i$  to the order of the low-energy theorem in units of  $e^2$ . The amplitudes  $A_3$ ,  $A_7$  and  $A_8$  are zero at this order. The second and third column refer to the negative- and positive-frequency contribution (Z-diagrams and ordinary diagrams) of the covariant calculation at second-order perturbation theory. The positive-frequency part of the covariant calculation is identical with the result of the effective Hamiltonian resulting from a direct Pauli reduction. The fourth column contains the additional part due to  $H_B$  in order to make the effective Hamiltonian gauge-invariant. The fifth and sixth column refer to the contact and non-contact terms of the Foldy-Wouthuysen calculation in second-order perturbation theory.



amplitude	covariant calculation		FW calculation in s. o. p. t.	
	negative	positive	contact	non-contact
$A_1$	$-\frac{\omega^2(1-\cos(\theta))}{2M^3} + \frac{\omega^2\kappa^2}{4M^3}$	$-\frac{\omega^2\kappa(1+\kappa)}{2M^3}$	$-\frac{\omega^2(1-\cos(\theta))}{2M^3} + \frac{\omega^2(1+\kappa+\kappa^2)}{4M^3}$	$-\frac{\omega^2(1+\kappa)(1+2\kappa)}{4M^3}$
$A_3$	$-\frac{\omega^2}{4M^3}$	$\frac{\omega^2(1+\kappa)^2 \cos(\theta)}{4M^3}$	$-\frac{\omega^2}{4M^3}$	$\frac{\omega^2(1+\kappa)^2 \cos(\theta)}{4M^3}$
$A_5$	$-\frac{\omega^2}{4M^3}$	$\frac{\omega^2(1+\kappa+\kappa^2)}{4M^3}$	$-\frac{\omega^2}{4M^3} - \frac{\omega^2\kappa}{8M^3}$	$\frac{\omega^2(2+3\kappa+2\kappa^2)}{8M^3}$
$A_6$	$-\frac{\omega^2}{4M^3}$	$\frac{\omega^2(1+\kappa+\kappa^2)}{4M^3}$	$-\frac{\omega^2}{4M^3} - \frac{\omega^2\kappa}{8M^3}$	$\frac{\omega^2(2+3\kappa+2\kappa^2)}{8M^3}$
$A_7$	$-\frac{\omega^2\kappa}{4M^3}$	0	$-\frac{\omega^2\kappa}{4M^3}$	0
$A_8$	$-\frac{\omega^2\kappa}{4M^3}$	0	$-\frac{\omega^2\kappa}{4M^3}$	0

**Table2: Compton Scattering amplitudes**

Contributions to the amplitudes  $A_i$  beyond the low-energy theorem to order  $\omega^2/M^3$  in units of  $e^2$ . The amplitudes  $A_2$  and  $A_4$  are zero at this order. Note that we have not constructed a Hamiltonian  $H_B$ .